Maxwell Equations without a Polarization Field

using a paradigm from biophysics

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ABSTRACT

Electrodynamics is almost always written using a polarization vector field to describe the response of matter to an electric field, or more specifically, to describe the change in distribution of charges as an electric field is applied or changed. This approach does not allow unique specification of a polarization field from measurements of the electric and magnetic fields and electrical current.

Many polarization fields will produce the same electric and magnetic fields, and current, because only the divergence of the polarization enters Maxwell's first equation, relating charge and electric field. The curl of any function can be added to a polarization field without changing the electric field at all. The divergence of the curl is always zero. Models of structures that produce polarization cannot be uniquely determined from electrical measurements for the same reason. Models must describe charge distribution not just distribution of polarization to be unique.

I propose a different approach, using a different paradigm to describe field dependent charge, i.e., to describe the phenomena of polarization. I propose an operational definition of polarization that has worked well in biophysics where a field dependent, time dependent polarization provides the gating current that makes neuronal sodium and potassium channels respond to voltage. The operational definition has been applied successfully to experiments for nearly fifty years. Estimates of polarization have been computed from simulations, models, and theories using this definition and they fit experimental data quite well.

I propose that the same operational definition be used to define polarization charge in experiments, models, computations, theories, and simulations of other systems. Charge movement needs to be computed from a combination of electrodynamics and mechanics because 'everything interacts with everything else'.

The classical polarization field need not enter into that treatment at all.

INTRODUCTION

Polarization has a central role in electrodynamics. Faraday and Maxwell thought all charge depends on the electric field. All charge would then be polarization.

Maxwell used the $\mathbf{D}$ and $\mathbf{P}$ fields as fundamental dependent variables. Charge only appeared as polarization, usually over-approximated by a dielectric constant ε_r that is a single real positive number. Charge independent of the electric field was not included, because the electron had not been discovered: physicists at Cambridge University (UK) did not think that charge could be independent of the electric field. The electron was discovered some decades later, in Cambridge, ironically enough [1, 2][1]. It became apparent to all that the permanent charge of an electron is a fundamental source of the electric field. The electron and permanent charge must be included in the equations defining the electric field, e.g., eq. (3) & eq. (6).

For physicists today, the fundamental electrical variable is the $\mathbf{E}$ field that describes the electric force on an infinitesimal test charge. $\mathbf{D}$ and $\mathbf{P}$ fields are auxiliary derived fields that many textbooks think unnecessary, at best [5-10].

THEORY

Maxwell's first equation for the composite variable $\mathbf{D}$ relates the 'free charge' $\boldsymbol{\rho}_f(x, y, z|t)$, units cou/m^3, to the sum of the electric field $\mathbf{E}$ and polarization $\mathbf{P}$. It is usually written as

$$\mathbf{div}\ \mathbf{D}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}|\boldsymbol{t}) \ = \ \boldsymbol{\rho}_{\boldsymbol{f}}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}|\boldsymbol{t}) \tag{1}$$

$$\mathbf{D}(x, y, z|t) \triangleq \ \varepsilon_0\, \mathbf{E}(x, y, z|t) + \mathbf{P}(x, y, z|t) \tag{2}$$

The physical variable $\mathbf{E}$ that describes the electric field is not visible in the classical formulation eq. (1). Maxwell embedded polarization in the very definition of the dependent variable $\mathbf{D} \triangleq \ \varepsilon_0\, \mathbf{E} + \mathbf{P}$. ε_0 is the electrical constant, sometimes called the 'permittivity of free space'. Polarization is described by a vector field $\mathbf{P}$ with units of dipole moment per volume, cou-m/m^3, that can be misleadingly simplified to cou-m^{-2}. The charge $\boldsymbol{\rho}_{\boldsymbol{f}}$ cannot depend on $\mathbf{D}$ or $\mathbf{E}$ in traditional formulations and so $\boldsymbol{\rho}_{\boldsymbol{f}}$ is a permanent charge.

[1] Thomson's monograph [3] "intended as a sequel to Professor Clerk-Maxwell's Treatise on electricity and magnetism" does not mention charge, as far as I can tell. Faraday's chemical law of electrolysis was not known and so the chemist's 'electron' postulated by Richard Laming and defined by Stoney [4] was not accepted in Cambridge as permanent charge, independent of the electric field. It is surprising that the physical unit 'the Faraday' describes a quantity of charged particles unknown to Michael Faraday. Indeed, he did not anticipate the existence or importance of permanent charge on particles or elsewhere.

When Maxwell's first equation is written with $\mathbf{E}$ as the dependent variable, the source terms are $\boldsymbol{\rho}_f$ and the divergence of $\mathbf{P}$. **Maxwell's first equation** for $\mathbf{E}$ is

$$\varepsilon_0 \mathbf{div}\, \mathbf{E}(x,y,z|t) = \boldsymbol{\rho}_f(x,y,z|t) - \mathbf{div}\, \mathbf{P}(x,y,z|t) \tag{3}$$

$\mathbf{P}$ itself does not enter the equation. Only the divergence of $\mathbf{P}$ appears on the right hand side of the Maxwell equation for $\mathbf{E}(x,y,z|t)$, eq. (3). $\mathbf{P}$ does not have the units of charge and should not be called the 'polarization charge'.

$\mathbf{D}(x,y,z|t)$ and the polarization $\mathbf{P}(x,y,z|t)$ are customarily over-approximated in classical presentations of Maxwell's equations: the polarization is assumed to be proportional to the electric field, independent of time.

$$\mathbf{P}(x,y,z|t) \triangleq (\varepsilon_r - 1)\varepsilon_0\, \mathbf{E}(x,y,z|t) \tag{4}$$

$$\mathbf{D}(x,y,z|t) \triangleq \varepsilon_r \varepsilon_0 \mathbf{E}(x,y,z|t) \tag{5}$$

The proportionality constant $(\varepsilon_r - 1)\varepsilon_0$ involves the dielectric constant ε_r which must be a single real positive number if the classical form of the Maxwell equations is taken as an exact mathematical statement of a system of partial differential equations. If ε_r is generalized to depend on time, or frequency, or the electric field, the form of the Maxwell equations change. If ε_r is generalized, traditional equations cannot be taken literally as a mathematical statement of a boundary value problem. They must be changed to accommodate the generalization.

1) Polarization and thus ε_r—however defined—depend on time or frequency in complex ways in all matter [11-16]. Many of the most interesting applications of electrodynamics arise from the dependence of polarization and ε_r on field strength.
2) ε_r should be taken as a constant only when experimental estimates, or theoretical models are not available, in my view.

It is difficult to imagine a physical system in which the electric field produces a change in charge distribution independent of time (see examples shown on p.12). The time range in which Maxwell's equations are used in the technology of our computers, smartphones, and video displays starts around 10^{-10} sec. The time range in which Maxwell's equations are used in biology start around 10^{-15} sec in simulations of the atoms that control protein function. The time range in which Maxwell's equations are used to design and operate the synchrotrons that generate x-rays (time scale $\sim 10^{-19}$ sec) to determine protein structure is very much faster than that, something like 10^{-23} sec.

A dielectric constant ε_r, independent of time is an inadequate over-approximation in many cases of practical interest today.

Despite these difficulties, **Maxwell's first equation** for $\mathbf{E}$

$$\varepsilon_r \varepsilon_0 \mathbf{div}\, \mathbf{E}(x,y,z|t) = \boldsymbol{\rho}_f(x,y,z|t) \tag{6}$$

is often written using the dielectric constant ε_r to describe polarization, without mention of the over-approximation involved.

RESULTS

Ambiguities in the traditional formulation. Equations (6) and (3) are ambiguous in an important way. They do not mention the shape or boundaries of the regions in question. In fact, if $\mathbf{P}$ varies from region to region, but is constant within each region, charge accumulates at the boundaries, and is absent within the region: when $\mathbf{P}$ is constant, $\mathbf{div}\ \mathbf{P} = 0$.

Such boundary charges are important in almost any system of dielectrics. Dielectric boundary charges have a particular role in biological systems, see Appendix on Proteins p.14 and [17].

Most of the properties of dielectric rods studied by Faraday—and predecessors going back to Benjamin Franklin, if not earlier—arise from the dielectric boundary charges. Textbooks typically spend much effort teaching why polarization charge appears on dielectric boundaries in systems with constant $\mathbf{P}$ where $\mathbf{div}\,\mathbf{P} = 0$ (e.g., Ch. 6 of [7]). Students wonder why regions without polarization charge have polarization charge on boundaries.

A general principle is at work here: a field equation in itself—like eq. (3) and (6) that are partial differential equations without boundary conditions—is altogether insufficient to specify an electric field. A model is needed that has boundary conditions, an explicit structure and describes the spatial variation of $\mathbf{P}$. Without specifying boundary conditions (defined explicitly in specific structures), using $\mathbf{P}$ in eq. (3) is ambiguous and confusing.

Indeed, using $\mathbf{P}$ without boundary conditions is so incomplete that it might be called incorrect.

$\mathbf{P}$ is not unique. The general nature of the ambiguity becomes clear once one realizes that:

Adding $\mathbf{curl}\ \widetilde{\mathbb{P}}(x, y, z|t)$ (7)

to $\mathbf{P}(x, y, z|t)$ in Maxwell's first equation, eq. (3)

changes nothing

because

$$\mathbf{div}\ \mathbf{curl}\ \widetilde{\mathbb{P}}(x, y, z|t)\ \equiv 0\ ; \tag{8}$$

see [18, 19]

The ambiguity in $\mathbf{P}$ means that any model $\mathbf{P}_{\boldsymbol{model}}(x, y, z|t)$ of polarization can have $\mathbf{curl}\ \widetilde{\mathbb{P}}(x, y, z|t)$ added to it, without making any change in the $\mathbf{div}\ \mathbf{P}(x, y, z|t)$ in Maxwell's first equation eq.(3), or its over-approximated version eq. (6). In other words, the polarization $\mathbf{div}\ \mathbf{P}(x, y, z|t)$ in Maxwell's first equation eq. (3) or (6) does not provide a unique structural model of polarization $\mathbf{P}_{\boldsymbol{model}}(x, y, z|t)$.

Any structural model can be modified by adding a polarization $\widetilde{\mathbf{P}}(x, y, z|t) \triangleq \mathbf{curl}\ \widetilde{\mathbb{P}}(x, y, z|t)$ to its representation of polarization without changing electrical properties at all.

Models of the polarization $\mathbf{P}^{\mathbf{1}}_{\boldsymbol{model}}$ and $\mathbf{P}^{\mathbf{2}}_{\boldsymbol{model}}$ of the same structure written by different authors may be strikingly different but they can give the same electrical results. If the models differ by the curl of a vector field, they will give the same result in the Maxwell equations even though the models can appear to be very different. The $\mathbf{curl}\ \widetilde{\mathbb{P}}(x, y, z|t)$ field can be quite complex and hard to recognize in a model. The two models $\mathbf{P}^{\mathbf{1}}_{\boldsymbol{model}}$ and $\mathbf{P}^{\mathbf{2}}_{\boldsymbol{model}}$ produce the same

charge distribution $\mathbf{div}\,\mathbf{P}^{\mathbf{1}}_{\boldsymbol{model}}$ and $\mathbf{div}\ \mathbf{P}^{\mathbf{2}}_{\boldsymbol{model}}$ in Maxwell's first equation eq. (3) and so they cannot be distinguished by measurements of electric field $\mathbf{E}(x,y,z|t)$, magnetic fields $\mathbf{B}(x,y,z|t)$, and electrical current $\mathbf{J}_{\boldsymbol{total}}$ (see eq. (11).

The P field is arbitrary. It is not surprising then that the structural models analyzed in detail by Purcell and Morin [5] are not unique, see p. 500 – 507.

Purcell and Morin are not guilty of hyperbole—indeed they may be guilty of understatement—when they say "The concept of polarization density $\mathbf{P}$ is more or less arbitrary" (slight paraphrase of [5], p. 507) and the $\mathbf{D}$ field is "is an artifice that is not, on the whole, very helpful" [5], p. 500.

The classical approach criticized by Purcell and Morin [5] does not allow unique specification of a polarization field $\mathbf{P}(x,y,z|t)$ from measurements of the electric $\mathbf{E}(x,y,z|t)$ and magnetic fields $\mathbf{B}(x,y,z|t)$, and electrical current $\mathbf{J}_{\boldsymbol{total}}$ (see eq. (11).

It seems clear that most formulations of electrodynamics of dielectrics in classical textbooks are "more or less arbitrary". An arbitrary formulation is not a firm foundation on which to build a theory of electrodynamics. See the Appendix p. 14 for a discussion of polarization in proteins in particular.

Maxwell First Equation, updated

$$\mathbf{div}\ \varepsilon_0\mathbf{E}(x,y,z|t)\ = \boldsymbol{\rho}_Q(x,y,z|t;\mathbf{E}) \tag{9}$$

Here $\boldsymbol{\rho}_Q(x,y,z|t;\mathbf{E})$ **describes all charge whatsoever**, no matter how small or fast or transient, including what is usually called dielectric charge and permanent charge, as well as charges driven by other fields, like convection, diffusion or temperature. Updated formulations of the Maxwell equations [13, 20] avoid the problems produced by ambiguous $\mathbf{P}$ and over-simplified ε_r.

Flow. Most applications of electrodynamics involve flow. We are interested in the flux of charges $\boldsymbol{\rho}_Q$ as well as their density and so I turn to Maxwell's second equation that describes current. It is understandable that Maxwell—and his Cambridge contemporaries and followers—had difficulty understanding current flow when their models did not include permanent charge, electrons or their motions.

Maxwell's extension of Ampere's law describes the special properties of current flow $\mathbf{J}_{total}$ (eq. (11) that make it so different from the flux of matter. Maxwell's field equations include the ethereal current $\varepsilon_0\,\partial\mathbf{E}/\partial t$ that makes the equations resemble those of a perfectly incompressible fluid. Maxwell's field equations describe the incompressible flow $\mathbf{J}_{total}$ over a dynamic range of something like 10^{16}, safely accessible within laboratories. The dynamic range is much larger if one includes the interior of stars, and the core of galaxies in which light is known to follow the same equations of electrodynamics as in our laboratories.

Maxwell's field equations are different from material field equations (like the Navier Stokes equations) because they are meaningful and valid universally [21], both in a vacuum devoid of mass and matter and within and between the atoms of matter [13]. The ethereal current $\varepsilon_0\,\partial\mathbf{E}/\partial t$ responsible for the special properties of Maxwell's equations arises from the Lorentz (un)transformation of charge. Charge does ***not*** vary with velocity, unlike mass, length, and time, all of which change dramatically as velocities approach the speed of light, strange as that seems.

This topic is explained in any textbook of electrodynamics that includes special relativity. Feynman's discussion of '*The Relativity of Electric and Magnetic Fields*' was an unforgettable revelation to me as a student [6], Section 13-6: an observer moving at the same speed as a stream of electrons sees zero current, but the forces measured by that observer are the same as the forces measured by an observed who is not moving at all. The moving observer describes the force as an electric field $\mathbf{E}(x, y, z|t)$. The unmoving observer describes the force as a magnetic field $\mathbf{B}(x, y, z|t)$. The observable forces are the same, whatever they are called, according to the principal and theory of relativity.[2]

The ethereal current reveals itself in magnetic forces which have no counterpart in material fields. The ethereal current is apparent in the daylight from the sun, that fuels life on earth, and in the night light from stars that fuels our dreams as it decorates the sky. The ethereal current is the term in the Maxwell equations that produces propagating waves in a perfect vacuum like space.

Magnetism B

defined by

Maxwell's Ampere Law

Maxwell's Second Equation

$$\frac{1}{\mu_0}\,\mathbf{curl}\,\mathbf{B} = \mathbf{J}_Q + \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} \tag{10}$$

$$\mathbf{J}_{total} \triangleq \mathbf{J}_Q + \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} \tag{11}$$

$$\frac{1}{\mu_0}\,\mathbf{curl}\,\mathbf{B} = \mathbf{J}_{total} \tag{12}$$

Note that $\mathbf{J}_Q$ includes the movement of all charge with mass, no matter how small, rapid or transient. It includes the movements of charge classically approximated as the properties of an ideal dielectric. It describes all movements of the charge described by $\boldsymbol{\rho}_Q(x, y, z|t; \mathbf{E})$; $\boldsymbol{\rho}_f$ is one of the components of $\boldsymbol{\rho}_Q$.

Indeed, $\mathbf{J}_Q$ can be written in terms of $\mathbf{v}_Q$ the velocity of mass with charge. In simple cases, such as a plasma of ions each with charge $\mathbf{Q}_Q$

$$\mathbf{J}_Q = \mathbf{v}_Q \mathbf{Q}_Q \mathbf{N}_Q \tag{13}$$

where $\mathbf{Q_Q}$ is the charge per particle and $\mathbf{N}_Q$ is the number density of particles. Note that sets of fluxes $\mathbf{J}_Q^i$, velocities $\mathbf{v}_Q^i$, charges $\mathbf{Q}_{Q,}^i$ number densities $\mathbf{N}_Q^i$, and charge densities $\boldsymbol{\rho}_Q^i$ are needed to keep track of each elemental species i of particles in a mixture. Plasmas are always mixtures because they must contain both positive and negative particles to keep electrical forces within safe bounds, as determined by (approximate) global electroneutrality.

[2] The principal and theory of relativity are confirmed to many significant figures every day in the GPS (global positioning systems) software of the map apps on our smartphones, and in the advanced photon sources (synchrotrons) that produce x-rays to determine the structure of proteins.

In other cases, more complex than plasmas, $\mathbf{J}_Q$ and $\mathbf{Q}_Q$ are related to material properties in more subtle ways. For example, the Maxwell equations do not describe charge and current driven by other fields, like convection, diffusion, or temperature. They do not describe constraints imposed by boundary conditions and mechanical structures. Those must be specified separately. If the other fields, structures, or boundary conditions involve matter with charge, they will respond to changes in the electric field. The other fields and constraints thus contribute to the phenomena of polarization and must be included in a description of it, as we shall discuss further below in the examples shown on p. 12. The theory of complex fluids can provide examples that deal with such cases, spanning scales, connecting micro (even atomic) structures with macro phenomena.

The charge density $\boldsymbol{\rho_Q}$ and current $\mathbf{J}_{\boldsymbol{total}}$ can be parsed into components in many ways, some helpful in one historical context, some in another. Ref. [12, 13, 20, 22-27] define and explore those representations in tedious detail. Simplifying those representations led to the treatment in this paper.

Conservation of Mass with Charge and Conservation of Current

Maxwell's Ampere's law implies two equations of great importance and generality.

First, it implies a continuity equation that describes the **conservation of charge with mass**. The continuity equation is the relation between the flux of charge with mass and density of charge with mass.

Second, it **implies conservation of total current**.

Derivation: Take the divergence of both sides of eq. (10), use $\mathbf{div\ curl} = \mathbf{0}$ [18, 19], and get

$$\mathbf{div}\ \mathbf{J}_Q = \mathbf{div}\left(-\varepsilon_0 \frac{\partial \mathbf{E}}{\partial t}\right) = -\varepsilon_0 \frac{\partial}{\partial t}\ \mathbf{div}\,\mathbf{E} \tag{14}$$

if we interchange time and spatial differentiation

But we have a relation between $\mathbf{div}\,\mathbf{E}$ and charge $\boldsymbol{\rho}_Q$ from Maxwell's first equation, eq. (9), so the result is the

Maxwell Continuity Equation

that describes the conservation of mass with charge

$$\mathbf{div}\ \mathbf{J}_Q = -\varepsilon_0\ \frac{\partial \boldsymbol{\rho}_Q}{\partial t} \tag{15}$$

$$\mathbf{div}\left(\mathbf{v}_Q \mathbf{Q}_Q \mathbf{N}_Q\right) = -\varepsilon_0\ \frac{\partial \boldsymbol{\rho}_Q}{\partial t} \tag{16}$$

Note that sets of fluxes $\mathbf{J}_Q^i$ and sets of charge densities $\boldsymbol{\rho}_Q^i$ are needed to keep track of each elemental species i of particles in a mixture, along with sets of velocities $\mathbf{v}_Q^i$, charges $\mathbf{Q}_{Q,}^i$ and number densities $\mathbf{N}_Q^i$, as described near eq. (13).

Derivation: Taking the divergence of both sides of Maxwell's Second law eq. (10) yields

Conservation of Total Current

$$\mathbf{div}\,\mathbf{J}_{total} \triangleq \mathbf{div}\left(\mathbf{J}_Q + \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t}\right) = 0 \tag{17}$$

$$\mathbf{div}\,\mathbf{J}_{total} = 0 \tag{18}$$

or

$$\mathbf{div}\,\mathbf{J}_{total} \triangleq \mathbf{div}\left(\mathbf{v}_Q \mathbf{Q}_Q \mathbf{N}_Q \mathbf{J}_Q + \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t}\right) = 0 \tag{19}$$

Conservation of current in one dimensional systems. One dimensional systems are of great importance despite, or because of their simplicity. The design of one dimensional systems is relatively easy. Their dimensionality rules out spatial singularities. Systems are more robust when steep slopes and infinities are not present to create severe sensitivity.

Branched one dimensional systems describe the electronic networks and circuits of our technology. Branched one dimensional systems describe the metabolic pathways of biological cells that make life possible. Branched one dimensional systems can be described accurately by a simple generalization of Kirchhoff's law: all the $\mathbf{J}_{total}$ that flows into a node must flow out [20, 24-26].

Unbranched one dimensional systems include the diodes of electronic technology and the ion channels of biological cells which are crucial components of technology and life.

Conservation of current in series systems. Unbranched one dimensional systems have components in series, each with its own current voltage relation arising from its microphysics. In a series one dimensional system, the total current $\mathbf{J}_{total}$ is equal everywhere at any time in every location no matter what the microphysics of the flux $\mathbf{J}_Q$ of charge with mass. Maxwell's equations ensure that $\varepsilon_0\,\partial\mathbf{E}/\partial t$, etc., take on the values at every location and every time needed to make the total currents $\mathbf{J}_{total}$ equal everywhere. An example is described in detail near Fig. 2 of [25].

There is no spatial dependence of total current in a series one dimensional system. No spatial variable or derivative is needed to describe total current in such a system [27], although of course spatial variables are needed to describe the flux $\mathbf{J}_Q$ of charge with mass, or the electrical current $\mathbf{Q}_Q^i\,\mathbf{J}_{total}^i$ of individual elemental species, or to describe the velocities, charge, and number densities $\mathbf{v}_Q$, $\mathbf{Q}_Q$, $\boldsymbol{\rho}_Q$, and $\mathbf{N}_Q$.

It is important to realize that the flux of charge with mass $\mathbf{J}_Q$ is not conserved. In fact, $\mathbf{div}\,\mathbf{J}_Q = \mathbf{div}\left(\mathbf{v}_Q \mathbf{Q}_Q \mathbf{N}_Q\right)$ supplies the flow of charge that is the current $\partial\boldsymbol{\rho}_Q\,/\partial t$ necessary to change $\mathbf{div}\,(\varepsilon_0\,\partial\mathbf{E}/\partial t)$ as described by the following continuity equation. Charges can

accumulate. $\mathbf{J}_Q$ can accumulate as $\mathbf{Q}_Q$. Total current $\mathbf{J}_{total}$ cannot, not al all, not anywhere ornot any time, when or where Maxwell's equations are valid.

$$\mathbf{div}\,\mathbf{J}_Q = \mathbf{div}\,\varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} = \frac{\partial}{\partial t}\mathbf{div}\,(\varepsilon_0 \mathbf{E}) = \frac{\partial \boldsymbol{\rho}_Q}{\partial t} \tag{20}$$

Because conservation of total current applies on every time and space scale, including those of thermal motion, the properties of $\mathbf{J}_Q$ differ a great deal from the properties of $\mathbf{J}_{total}$. For example, in one dimensional channels, the material flux $\mathbf{J}_Q$ can exhibit all the complexities of a function of infinite variation, without a time derivative, like a trajectory of a Brownian stochastic process, that reverses direction an uncountably infinite number of times in any interval, however small, while the electrical current $\mathbf{J}_{total}$ will be spatially uniform [27], strange as that seems. The fluctuations of $\varepsilon_0\,\partial\mathbf{E}/\partial t$ and other variables are exactly what is needed to smooth the bizarrely infinite fluctuations of $\mathbf{J}_Q$ into the spatially uniform $\mathbf{J}_{total}$.

DISCUSSION

How is the phenomenon of polarization included in the updated version of the Maxwell equations eq. (9) & eq. (12)? First, we need a general paradigm to define polarization, even when dielectrics are far from ideal, time and frequency dependent, and voltage dependent as well.

Biophysical Paradigm. I propose adopting the operational definition of 'gating current' used to define nonlinear time and voltage dependent polarization by biophysicists since 1972 [28-30]. A community of scholars has studied the nonlinear currents that control the opening of voltage sensitive protein channels for nearly fifty years , inspired by [31]. They have developed protocols that may be as useful in other systems, as they have been in biophysics.

The basic idea is to apply a set of step functions of potential and observe the currents that flow. The currents observed are transients that decline to a steady value, often to near zero after a reasonable (biologically relevant) time. The measured currents are perfectly reproducible. If a pulse is applied, the charge moved (the integral of the current) can be measured when the voltage step is applied. The integration goes on until t_1 when the current i_{leak} is nearly independent of time, often nearly zero. That integral is called the **ON** charge $\mathbf{Q_{ON}}$.

When the voltage is returned to its initial value (the value that was present before the **ON** pulse), another current is observed that often has quite different time course [28-30]. The integral of that current is the **OFF** charge $\mathbf{Q_{OFF}}$.

This gating current depends on the voltage before the step. It also depends ***separately*** on the voltage after the step, although Fig. 1 does not illustrate the dependence documented in the literature [28-30]. The voltage and time dependence defines the molecular motions underlying the gating current [32-34]. If the **ON** charge is found experimentally to equal the **OFF** charge, for

a variety of pulse sizes and range of experimental conditions, the current is said to arise in a nonlinear (i.e., voltage dependent) polarization capacitance and is interpreted as the movement of charged groups in the electric field that move to one location after the **ON** pulse, and return

Figure 1

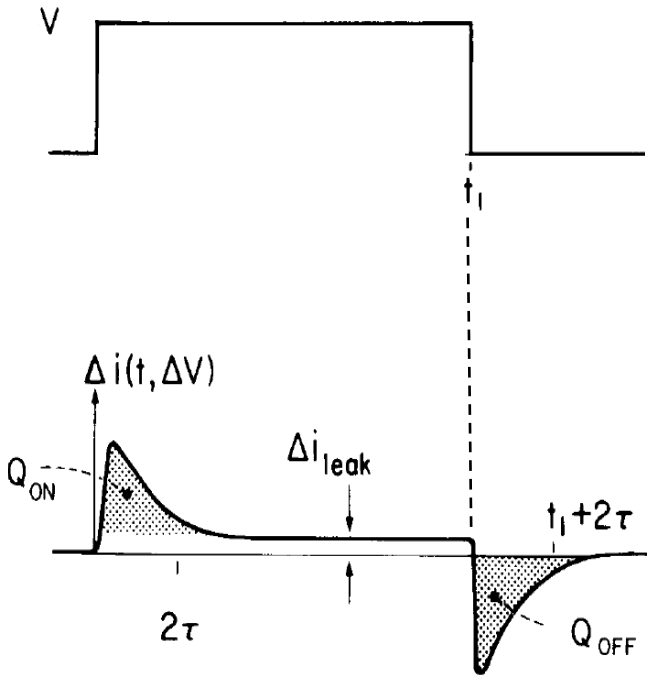

Fig. 1 shows the response to a step function change in potential and the charges measured that are proposed as an operational definition of polarization.

to their original location following the **OFF** pulse. The charge is called 'gating charge' and the current that carries the charge is called 'gating current'.

The current observed in the set up is equal to the current carried by the charged groups remote from the boundaries of the setup because the setup is designed to be an unbranched one dimensional circuit with everything in series. In a one dimensional series setup the total current is equal everywhere in the series system at any one time, even though the total current varies significantly with time. The equality of current can easily be checked in the experiment. The spatial equality of current needs to be checked in simulations as in [32-34].

If the currents reach a steady value independent of time, but not equal to zero, as in Fig. 1, the steady current i_{leak} is considered to flow in a resistive path that is time independent, but

perhaps voltage dependent, in parallel with the device in which the gating charges $\mathbf{Q_{ON}}$ and $\mathbf{Q_{OFF}}$ flow. If the current does not reach a steady value, or if the areas are not equal, the currents are not considered 'capacitive' and are interpreted as those through a time and voltage dependent 'resistor'. It is important to check the currents through the resistive path by independent methods to see if they are time independent, by blocking the path with drugs, or one way or the other. If the resistive currents are not time independent, the definition of $\mathbf{Q_{ON}}$ and $\mathbf{Q_{OFF}}$ in Fig. 1 needs to be changed.

Clearly, this approach will only work if step functions can reveal all the properties of the system. If the underlying mechanisms depend on the rate of change of velocity, step functions are clearly insufficient.

Much work has been done showing that step functions are enough to understand the voltage dependent mechanisms in the classical action potential of the squid axon [35-37], starting with [38], Fig. 10 and eq. 11. Hodgkin kindly explained the significance of this issue to colleagues, including the author (around 1970). He explained the possible incompleteness of step function measurements: if sodium conductance had a significant dependence on $\partial V/\partial t$, the action potential computed from voltage clamp data would differ from experimental measurements. He mentioned that this possibility was an important motivation for Huxley's heroic hand integration [31] of the Hodgkin Huxley differential equations. Huxley confirmed this in a separate personal communication, Huxley to Eisenberg. Those computations and many papers since [35-37] have shown that voltage clamp data (in response to steps) is enough to predict the shape and propagation of the action potential in nerve and skeletal muscle. It should be clearly understood that such a result is not available for biological systems in which the influx of Ca^{++} drives the action potential and its propagation [39].

The conductance of the voltage activated calcium channel has complex dependence on the current through the channel because the concentration of Ca^{++} in the cytoplasm is so low ($\sim 10^{-8}$M at rest) that the current almost always changes the local concentration near the cytoplasmic side of the channel. Current through the channel changes the local concentration. The local concentration changes the gating and selectivity characteristics of the channel protein, as calcium ions are prone to do at many physical and biological interfaces. It seems unlikely that the resulting properties can be described by the same formalism [31] used for voltage controlled sodium and potassium channels of nerve and skeletal muscle. That formalism uses variables that depend on membrane potential and not membrane current because it was evident to Cole [40] and Hodgkin [41-43] that neuronal action potentials were essentially voltage dependent, not current dependent. There may of course be other reasons the formalism [31] is inadequate. Experiments are needed to show that responses to steps of voltage allow computation of a calcium driven action potential.

Polarization defined in theories and simulations. The polarization protocol described here can be applied to models and simulations of polarization as well as experiments. Indeed, the

operational definition of polarization has been applied even when theories [32] or simulations are enormously complicated by atomic detail including the individual motions of thousands of atoms [33, 34].

Does the estimated polarization equal $\mathbf{P}$? The question of general interest is how does the polarization defined this way correspond to the polarization $\mathbf{P}$ in the classical formulation of the Maxwell equations eq. (3)?

Polarization cannot be defined in general. The variety of possible responses of matter to a step of potential prevents a general answer.

Indeed, a main point of this paper is that ***polarization must be defined by a protocol in a specific setting***. It cannot be defined in general. The possible motions of mass and mass with charge are too many to permit a general definition of polarization. Every possible motion of mass (with charge, including rotations and translations and changes of shape) would produce a polarization. Polarization currents can be as complicated as the motions of matter.

Insight can be developed into various kinds of polarization by constructing 'toy' models of classical systems, applying the operational definition of polarization, and understanding the resulting estimates of polarization currents (that are called 'gating currents' in the biophysical literature).

Those models must specify the mechanical variables $\mathbf{v}_{Q,}\ \mathbf{Q}_Q, \boldsymbol{\rho}_Q$ and $\mathbf{N}_Q$ (or their equivalent) and solve the field equations of mechanics along with the Maxwell equations. Indeed, toy problems are examples that may help develop insight:

(1) simple electro-mechanical models, like a charged mass on a spring with damping.

(2) ideal gases of permanently charged particles, i.e., biological and physical plasmas.

(3) ideal gases of dipoles (point and macroscopic), quadrupoles, and mixtures of dipoles and quadrupoles, that rotate and translate while some are attached by bonds that vibrate (see (1)). These mixtures should provide decent representations of liquid water in ionic solutions, if they include a background dielectric, even if the dielectric is over-approximated with a single dielectric constant ε_r.

(4) molecular models of ionic solutions that include water as a molecule. It is best to use models that are successful in predicting the activity of solutions of diverse composition and content and include water and ions as molecules of unequal nonzero size [44].

(5) classical models of impedance, dielectric .and molecular spectroscopy [16, 45-50].

(6) well studied systems of complex fluids, spanning scales, connecting micro (even atomic) structures with macroscopic functions.

These examples, taken together, will form a handbook of practical examples closely related to the classical approximations of dielectrics.

These problems have time dependent solutions except in degenerate, uninteresting cases. As stated in [20] on p. 13

> "It is necessary also to reiterate that ε_r is a single, real positive constant in Maxwell's equations as he wrote them and as they have been stated in many textbooks since then, following [51-53]. If one wishes to generalize ε_r so that it more realistically describes the properties of matter, one must actually change the differential equation (6) and the set of Maxwell's equations as a whole. If, to cite a common (but not universal) example, ε_r is to be generalized to a time dependent function (because polarization current in this case is a time dependent solution of a linear, often constant coefficient, differential equation that depends only on the local electric field), the mathematical structure of Maxwell's equations changes.
>
> [Perhaps it is tempting to take a short cut by simply converting ε_r into a function of time $\varepsilon_r(t)$ in Maxwell's equations, as classically written.] Solving the equations with a constant ε_r and then letting ε_r become a function of time creates a mathematical chimera that is not correct. The chimera is not a solution of the equations. [The full functional form, or differential equation for $\varepsilon_r(t)$ must be written and solved together with he Maxwell equations. This is a formidable task in any case, but becomes a formidable challenge if convection or electrodiffusion modify polarization, as well as the electric field.]
>
> Even if one confines oneself to sinusoidal systems (as in classical impedance or dielectric spectroscopy [11, 45, 54, 55]), one should explicitly introduce the sinusoids into the equations and not just assume that the simplified treatment of sinusoids in elementary circuit theory [56-60] is correct: it is not at all clear that Maxwell's equations— combined with other field equations (like Navier Stokes [61-78] or PNP = drift diffusion [66, 79-94]); [joined] with constitutive equations; and boundary conditions—always have steady state solutions in the sinusoidal case. They certainly do not always have solutions that are linear functions of just the electric field [95-98]."

It seems clear that the classical Maxwell equations with the over-approximated dielectric coefficient ε_r cannot emerge in the time dependent case. Of course, the classical Maxwell equations cannot emerge when polarization has a nonlinear dependence on the electric field, or depends on the global (not local) electric field, or depends on convection or electrodiffusion.

Indeed, in my opinion, when confronted with these models of polarization, the classical Maxwell equations will be seen as useful only when knowledge of the actual properties of polarization is missing.

A generalization of Maxwell's $\mathbf{P}$ may emerge from these examples that describes a wide enough range of systems to be useful, one imagines that Maxwell hoped $\mathbf{P}$ and $\mathbf{D}$ would.

Until then, one is left with

(1) bewilderingly complete measurements, over an enormous range of frequencies (e.g., [14]) of the dielectric properties and conductance of ionic solutions of varying composition and content. These measurements embarrass the theoretician with their diversity and complexity. They have not yet been captured in any formulas or programs less complicated than a look up table of all the results.

(2) computations of the motion of all charges on the atomic scale [33, 34], described by the field equations of mechanics and electrodynamics [32].

What should be done when little is known? Sadly, the actual properties of polarization are often unknown. Then, one is left with the over-approximated eq. (6) or nothing at all. Eq. (6) is certainly better than nothing: it is almost never useful to assume polarization effects contribute nothing to phenomena. Eq. (6) can be useful if it is used gingerly: toy models can usefully represent an idealized view of part of the real world.

In some cases, the toy models can be enormously helpful. They allow the design of circuits in our analog and digital electronic technology [99-102]. They allow the understanding of selectivity [44, 103-105] and current voltage relations of several important biological channel proteins in a wide range of solutions [44, 106-108]. In other cases—for example the description of ionic solutions with many components—they can be too unrealistic to be useful. Experiments and experience can tell how useful the toy model actually is in a particular case: pure thought usually cannot.

APPENDIX

$\mathbf{P}(x, y, z|t)$ in Proteins

Ambiguities in the meaning of the polarization field $\mathbf{P}(x, y, z|t)$ can cause serious difficulties in the understanding of protein function. The protein data bank contains 167,327 structures in atomic detail today (August 11, 2020) and the number is growing rapidly as cryo-electron microscopy is used more and more.

Protein structures are usually analyzed with molecular dynamics programs that assume periodic boundary conditions. Proteins are not periodic in their natural setting. It seems obvious that periodic systems cannot conserve total current $\mathbf{J}_{total}$ in general—or perhaps even in particular—as required by the Maxwell equations, see eq. (17). In other words, it is likely that molecular dynamics analyses of periodic structures do not satisfy the Maxwell equations, although almost all known physics does satisfy those equations.

It is also unlikely that standard programs of molecular dynamics compute electrodynamics of ***non***periodic systems correctly, despite their use of Ewald sums, with various conventions, and force fields (tailored to fit macroscopic, not quantum mechanical) data. Compare the exhaustive methods used to validate results in computational electronics [86] with those in the computation of electric fields in proteins.

The electrostatic and electrodynamic properties of proteins are of great importance. Many of the atoms in a protein are assigned permanent charge greater than $0.2\mathbf{e}$ in the force fields used in molecular dynamics, where $\mathbf{e}$ is the elementary charge, and these charges tend to

cluster in locations most important for biological function. Enormous densities of charge ($> 10\mathrm{M}$, sometimes much larger) are found in and near channels of proteins [44, 109-111] and in the 'catalytic active sites' [112] of enzymes. Such densities are also found near nucleic acids, DNA and all types of RNA and binding sites of proteins in general.

A feel for the size of electrostatic energies can be found from Coulomb's law between isolated charges (in an infinite domain without boundary conditions).

$$E_{cou} = \frac{560}{\varepsilon_r}\frac{q_i q_j}{r_{ij}} \tag{21}$$

Here E_{cou} is in units of the thermal energy RT, with gas constant R and absolute temperature T; charge q_i or q_j are in units of the elementary charge $\mathbf{e}$; and r_{ij} is in units of Angstroms $= 10^{-10}$ meters.

For water, with $\varepsilon_r \cong 80$, this becomes

$$E_{cou}(\text{water}) = 7\frac{q_i q_j}{r_{ij}}\text{; units RT} \tag{22}$$

For the pore of a channel, one can guess $\varepsilon_r \cong 10$ and then

$$E_{cou}(\text{channel: } \varepsilon_r \cong 10\ ) = 56\ \frac{q_i q_j}{r_{ij}}\text{; units RT} \tag{23}$$

Electrostatic energy has to be computed very accurately indeed to predict current voltage relations. Gillespie ([108] particularly in 'Supplemental Data') found that errors of energy of $0.05\ \mathrm{RT}$ produced significant changes in current voltage relations of the ryanodine receptor protein. Similar sensitivity is expected for any model of an ion channel or the active site of an enzyme or the binding site of a protein in which the underlying energetics are similar.

Accuracy of this sort is not claimed in most calculations of molecular or quantum dynamics involving ionic solutions. Typical accuracies claimed for quantum chemical calculations start around 2 RT and for molecular dynamics calculations around 0.5 RT, in my (limited) experience. However, reduced models of proteins allow calculations of the precision needed to deal with Gillespie's results, as much work demonstrates [106, 108, 113-116]. Reduced models use lower resolution representations drawn from the full detail atomic structure. Typically the accuracy of the reduced model itself cannot be calculated from first principles. But if the model fits a wide range of data, measured in solutions of different composition and contents with a single set of parameters, as does Gillespie's, the precision of the model is assured by the fit to the data itself [108].

Polarization must be accurately calculated to understand protein function. Polarization phenomena are as important as permanent charges. Charges that depend on the electric field are as important as the permanent charges analyzed in the last paragraphs (see [117] and references cited there). The enormous effort and investment in developing polarizable force fields [118] is an eloquent testimonial to the importance of polarization in biological and chemical applications.

The ambiguous nature of the $\mathbf{P}$ field means that $\mathbf{P}$ provides a poor guide to the importance of polarization in a particular protein. Identical electrodynamics will arise from structures that appear different, but only differ by $\mathbf{curl}\ \widetilde{\mathbb{P}}(x, y, z|t)$. Situations like this can produce confusion

and unproductive argument, because not all scientists—particularly structural biologists—realize the inherent unavoidable ambiguity of $\mathbf{div}\,\mathbf{P}$ or eq. (3)**.**

What is needed is a model of both the dynamics of mass and the electrodynamics of charge, that allows the unambiguous calculation of the response of the protein to an applied electric field. The combined dynamics of mass and electrodynamics of charge (that depends on the electric field) are the appropriate model of the polarization phenomena, not the classical $\mathbf{P}$ field.

Low resolution models may do surprisingly well provided they actually satisfy the Maxwell equations and conservation of current, avoiding periodic boundary conditions for the electric field in nonperiodic systems. Compare [32] and [33, 119].

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